

Asymptotic properties of Bernstein estimators on the simplex

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Abstract

In this paper, we study various asymptotic properties (bias, variance, mean squared error, mean integrated squared error, asymptotic normality, uniform strong consistency) for Bernstein estimators of cumulative distribution functions and density functions on the d -dimensional simplex. Our results generalize the ones in [Leblanc \(2012a\)](#) and [Babu et al. \(2002\)](#), which treated the case $d = 1$, and significantly extend those found in [Tenbusch \(1994\)](#) for the density estimators when $d = 2$. The density estimator (or smoothed histogram) is closely related to the Dirichlet kernel estimator from [Ouimet \(2020a\)](#), and can also be used to analyze compositional data.

Keywords: Bernstein estimators, simplex, cumulative distribution function estimation, density estimation, mean squared error, asymptotic normality, uniform strong consistency
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1. Introduction

The d -dimensional simplex and its interior are defined by

$$\mathcal{S} := \{\mathbf{x} \in [0, 1]^d : \|\mathbf{x}\|_1 \leq 1\} \quad \text{and} \quad \text{Int}(\mathcal{S}) := \{\mathbf{x} \in (0, 1)^d : \|\mathbf{x}\|_1 < 1\}, \quad (1.1)$$

where $\|\mathbf{x}\|_1 := \sum_{i=1}^d |x_i|$. For any cumulative distribution function F on \mathcal{S} , define the Bernstein polynomial of order m for F by

$$F_m^*(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} F(\mathbf{k}/m) P_{\mathbf{k},m}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{S}, \quad m \in \mathbb{N}, \quad (1.2)$$

where the weights are the following probabilities from the Multinomial(m, \mathbf{x}) distribution :

$$P_{\mathbf{k},m}(\mathbf{x}) := \frac{m!}{(m - \|\mathbf{k}\|_1)! \prod_{i=1}^d k_i!} \cdot (1 - \|\mathbf{x}\|_1)^{m - \|\mathbf{k}\|_1} \prod_{i=1}^d x_i^{k_i}, \quad \mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}. \quad (1.3)$$

The Bernstein estimator of F , denoted $F_{n,m}^*$, is the Bernstein polynomial of order m for the [empirical cumulative distribution function](#) $F_n(\mathbf{x}) := n^{-1} \sum_{j=1}^n \mathbb{1}_{(-\infty, \mathbf{x}]}(\mathbf{X}_j)$, where the random variables $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ are independent and F distributed. Precisely,

$$F_{n,m}^*(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} F_n(\mathbf{k}/m) P_{\mathbf{k},m}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{S}, \quad m, n \in \mathbb{N}. \quad (1.4)$$

Similarly, if F has a density function f , we define the Bernstein density estimator of f by

$$\hat{f}_{n,m}(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} \frac{m^d}{n} \sum_{i=1}^n \mathbb{1}_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]}(\mathbf{X}_i) P_{\mathbf{k},m-1}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{S}, \quad m, n \in \mathbb{N}, \quad (1.5)$$

where m^d is just a scaling factor, namely the inverse of the volume of the hypercube $(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]$.

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2. Results for the c.d.f. estimator $F_{n,m}^*$

Except for Theorem 2.7, we assume the following everywhere in this section :

Assumption.

- F is twice differentiable and its second order partial derivatives are (uniformly) continuous on \mathcal{S} . (2.1)

Proposition 2.1. Under assumption (2.1), we have, uniformly for $\mathbf{x} \in \mathcal{S}$,

$$F_m^*(\mathbf{x}) = F(\mathbf{x}) + m^{-1}B(\mathbf{x}) + o(m^{-1}), \quad (2.2)$$

as $m \rightarrow \infty$, where

$$B(\mathbf{x}) := \frac{1}{2} \sum_{i,j=1}^d (x_i \mathbb{1}_{\{i=j\}} - x_i x_j) \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}). \quad (2.3)$$

Theorem 2.2 (Bias and variance). Under assumption (2.1), we have, for $\mathbf{x} \in \text{Int}(\mathcal{S})$,

$$\text{Bias}[F_{n,m}^*(\mathbf{x})] = \mathbb{E}[F_{n,m}^*(\mathbf{x})] - F(\mathbf{x}) = m^{-1}B(\mathbf{x}) + o(m^{-1}), \quad (2.4)$$

$$\text{Var}(F_{n,m}^*(\mathbf{x})) = n^{-1}\sigma^2(\mathbf{x}) - m^{-1/2}n^{-1}V(\mathbf{x}) + \mathcal{O}_{\mathbf{x}}(m^{-1}n^{-1}), \quad (2.5)$$

as $m, n \rightarrow \infty$, where

$$\sigma^2(\mathbf{x}) := F(\mathbf{x})(1 - F(\mathbf{x})) \quad \text{and} \quad V(\mathbf{x}) := \sum_{i=1}^d \frac{\partial}{\partial x_i} F(\mathbf{x}) \sqrt{x_i(1 - x_i)/\pi}. \quad (2.6)$$

Remark 2.3. In Leblanc (2012a), the function $V(x)$ should be equal to $f(x)\sqrt{x(1-x)/\pi}$ instead of $f(x)\sqrt{2x(1-x)/\pi}$. The error is explained in the appendix and the estimates can easily be verified numerically. The same error also appears in the statements of Belalia (2016), since the proofs relied on the same estimates as Leblanc.

Corollary 2.4 (Mean squared error). Under assumption (2.1), we have, for $\mathbf{x} \in \text{Int}(\mathcal{S})$,

$$\begin{aligned} \text{MSE}(F_{n,m}^*(\mathbf{x})) &= n^{-1}\sigma^2(\mathbf{x}) - n^{-1}m^{-1/2}V(\mathbf{x}) + m^{-2}B^2(\mathbf{x}) \\ &\quad + \mathcal{O}_{\mathbf{x}}(n^{-1}m^{-1}) + o(m^{-2}). \end{aligned} \quad (2.7)$$

In particular, if $V(\mathbf{x}) \cdot B(\mathbf{x}) \neq 0$, the asymptotically optimal choice of m , with respect to MSE, is

$$m_{\text{opt}} = n^{2/3} \left[\frac{4B^2(\mathbf{x})}{V(\mathbf{x})} \right]^{2/3}, \quad (2.8)$$

in which case

$$\text{MSE}[F_{n,m_{\text{opt}}}^*(\mathbf{x})] = n^{-1}\sigma^2(\mathbf{x}) - n^{-4/3} \frac{3}{4} \left[\frac{V^4(\mathbf{x})}{4B^2(\mathbf{x})} \right]^{1/3} + o_{\mathbf{x}}(n^{-4/3}). \quad (2.9)$$

Theorem 2.5 (Mean integrated squared error). Under assumption (2.1), we have

$$\begin{aligned} \text{MISE}[F_{n,m}^*] &= n^{-1} \int_{\mathcal{S}} \sigma^2(\mathbf{x}) d\mathbf{x} - n^{-1}m^{-1/2} \int_{\mathcal{S}} V(\mathbf{x}) d\mathbf{x} + m^{-2} \int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x} \\ &\quad + o(n^{-1}m^{-1/2}) + o(m^{-2}). \end{aligned} \quad (2.10)$$

In particular, if $\int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x} > 0$, the asymptotically optimal choice of m , with respect to MISE, is

$$m_{\text{opt}} = n^{2/3} \left[\frac{4 \int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x}}{\int_{\mathcal{S}} V(\mathbf{x}) d\mathbf{x}} \right]^{2/3}, \quad (2.11)$$

in which case

$$\text{MISE}[F_{n,m_{\text{opt}}}^*] = n^{-1} \int_{\mathcal{S}} \sigma^2(\mathbf{x}) d\mathbf{x} - n^{-4/3} \frac{3}{4} \left[\frac{(\int_{\mathcal{S}} V(\mathbf{x}) d\mathbf{x})^4}{4 \int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x}} \right]^{1/3} + o(n^{-4/3}). \quad (2.12)$$

Theorem 2.6 (Asymptotic normality). Assume (2.1). For $\mathbf{x} \in \text{Int}(\mathcal{S})$ such that $0 < F(\mathbf{x}) < 1$, we have the following convergence in distribution :

$$n^{1/2}(F_{n,m}^*(\mathbf{x}) - F_m^*(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2(\mathbf{x})), \quad \text{as } m, n \rightarrow \infty. \quad (2.13)$$

In particular, Proposition 2.1 implies

$$n^{1/2}(F_{n,m}^*(\mathbf{x}) - F(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2(\mathbf{x})), \quad \text{if } n^{1/2}m^{-1} \rightarrow 0, \quad (2.14)$$

$$n^{1/2}(F_{n,m}^*(\mathbf{x}) - F(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(\lambda B(\mathbf{x}), \sigma^2(\mathbf{x})), \quad \text{if } n^{1/2}m^{-1} \rightarrow \lambda, \quad (2.15)$$

for any constant $\lambda > 0$.

For the next result, we use the notation $\|G\|_\infty := \sup_{\mathbf{x} \in \mathcal{S}} |G(\mathbf{x})|$ for any bounded function $G : \mathcal{S} \rightarrow \mathbb{R}$, and also

$$\alpha_n := (n^{-1} \log n)^{1/2} \quad \text{and} \quad \beta_{n,m} := \alpha_n \sqrt{\alpha_m}. \quad (2.16)$$

Theorem 2.7 (Uniform strong consistency). Let F be continuous on \mathcal{S} . Then, as $m, n \rightarrow \infty$,

$$\|F_{n,m}^* - F\|_\infty \longrightarrow 0 \quad \text{a.s.} \quad (2.17)$$

Assume further that F is differentiable and its partial derivatives are Lipschitz continuous on \mathcal{S} . Then, for all $m \geq 2$ such that $m^{-1} \leq \beta_{n,m} \leq \alpha_m$ (for example, $2n^{2/3}/\log n \leq m \leq n^2/\log n$ works), we have, as $m, n \rightarrow \infty$,

$$\|F_{n,m}^* - F_n\|_\infty = \mathcal{O}(\beta_{n,m}) \quad \text{a.s.} \quad (2.18)$$

In particular, for $m = n$, we have $\|F_{n,m}^* - F_n\|_\infty = \mathcal{O}(n^{-3/4}(\log n)^{3/4})$ a.s.

3. Results for the density estimator $\hat{f}_{n,m}$

For each result stated in this section, one of the following two assumptions will be used.

Assumptions.

- The density f is Lipschitz continuous on \mathcal{S} . (3.1)

- f is twice differentiable and its second order partial derivatives are (uniformly) continuous on \mathcal{S} . (3.2)

We denote the expectation of $\hat{f}_{n,m}(\mathbf{x})$ by

$$f_m(\mathbf{x}) := \mathbb{E}[\hat{f}_{n,m}(\mathbf{x})] = \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} m^d \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} P_{\mathbf{k},m}(\mathbf{x}). \quad (3.3)$$

Proposition 3.1. Under assumption (3.2), we have, uniformly for $\mathbf{x} \in \mathcal{S}$,

$$f_m(\mathbf{x}) = f(\mathbf{x}) + m^{-1}b(\mathbf{x}) + o(m^{-1}), \quad (3.4)$$

as $m \rightarrow \infty$, where

$$b(\mathbf{x}) := \sum_{i=1}^d \left(\frac{1}{2} - x_i\right) \frac{\partial}{\partial x_i} f(\mathbf{x}) + \frac{1}{2} \sum_{i,j=1}^d (x_i \mathbb{1}_{\{i=j\}} - x_i x_j) \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x}). \quad (3.5)$$

Theorem 3.2 (Bias and variance). We have, for $\mathbf{x} \in \text{Int}(\mathcal{S})$,

$$\mathbb{B}\text{ias}[\hat{f}_{n,m}(\mathbf{x})] = \mathbb{E}[\hat{f}_{n,m}(\mathbf{x})] - f(\mathbf{x}) = m^{-1}b(\mathbf{x}) + o(m^{-1}), \quad \text{assuming (3.2)}, \quad (3.6)$$

$$\mathbb{V}\text{ar}(\hat{f}_{n,m}(\mathbf{x})) = n^{-1}m^{d/2}\psi(\mathbf{x})f(\mathbf{x}) + \mathcal{O}_{\mathbf{x}}(n^{-1}m^{d/2-1/2}), \quad \text{assuming (3.1)}, \quad (3.7)$$

as $m, n \rightarrow \infty$, where

$$\psi(\mathbf{x}) := [(4\pi)^d x_1 x_2 \dots x_d (1 - \|\mathbf{x}\|_1)]^{-1/2}. \quad (3.8)$$

Corollary 3.3 (Mean squared error). Under assumption (3.2), we have, for $\mathbf{x} \in \text{Int}(\mathcal{S})$,

$$\text{MSE}(\hat{f}_{n,m}(\mathbf{x})) = n^{-1}m^{d/2}\psi(\mathbf{x})f(\mathbf{x}) + m^{-2}b^2(\mathbf{x}) + \mathcal{O}_{\mathbf{x}}(n^{-1}m^{d/2-1/2}) + o(m^{-2}). \quad (3.9)$$

In particular, if $f(\mathbf{x}) \cdot b(\mathbf{x}) \neq 0$, the asymptotically optimal choice of m , with respect to MSE, is

$$m_{\text{opt}} = n^{2/(d+4)} \left[\frac{4}{d} \cdot \frac{b^2(\mathbf{x})}{\psi(\mathbf{x})f(\mathbf{x})} \right]^{2/(d+4)}, \quad \text{with} \quad (3.10)$$

$$\text{MSE}[\hat{f}_{n,m_{\text{opt}}}] = n^{-4/(d+4)} \left[\frac{\frac{4}{d} + 1}{\left(\frac{4}{d}\right)^{\frac{4}{d+4}}} \right] \frac{(\psi(\mathbf{x})f(\mathbf{x}))^{4/(d+4)}}{(g^2(\mathbf{x}))^{-d/(d+4)}} + o_{\mathbf{x}}(n^{-4/(d+4)}), \quad (3.11)$$

and, more generally, if $n^{2/(d+4)}m^{-1} \rightarrow \lambda$ for some $\lambda > 0$, then

$$\text{MSE}[\hat{f}_{n,m}(\mathbf{x})] = n^{-4/(d+4)} [\lambda^{-d/2}\psi(\mathbf{x})f(\mathbf{x}) + \lambda^2b^2(\mathbf{x})] + o_{\mathbf{x}}(n^{-4/(d+4)}). \quad (3.12)$$

Theorem 3.4 (Mean integrated squared error). Under assumption (3.2), we have

$$\text{MISE}[\hat{f}_{n,m}] = n^{-1}m^{d/2} \int_{\mathcal{S}} \psi(\mathbf{x})f(\mathbf{x})d\mathbf{x} + m^{-2} \int_{\mathcal{S}} b^2(\mathbf{x})d\mathbf{x} + o(n^{-1}m^{d/2}) + o(m^{-2}). \quad (3.13)$$

In particular, if $\int_{\mathcal{S}} b^2(\mathbf{x})d\mathbf{x} > 0$, the asymptotically optimal choice of m , with respect to MISE, is

$$m_{\text{opt}} = n^{2/(d+4)} \left[\frac{4}{d} \cdot \frac{b^2(\mathbf{x})}{\psi(\mathbf{x})f(\mathbf{x})} \right]^{2/(d+4)}, \quad \text{with} \quad (3.14)$$

$$\text{MISE}[\hat{f}_{n,m_{\text{opt}}}] = n^{-4/(d+4)} \left[\frac{\frac{4}{d} + 1}{\left(\frac{4}{d}\right)^{\frac{4}{d+4}}} \right] \frac{(\int_{\mathcal{S}} \psi(\mathbf{x})f(\mathbf{x})d\mathbf{x})^{4/(d+4)}}{(\int_{\mathcal{S}} g^2(\mathbf{x})d\mathbf{x})^{-d/(d+4)}} + o_{\mathbf{x}}(n^{-4/(d+4)}), \quad (3.15)$$

and, more generally, if $n^{2/(d+4)}m^{-1} \rightarrow \lambda$ for some $\lambda > 0$, then

$$\text{MISE}[\hat{f}_{n,m}] = n^{-4/(d+4)} \left[\lambda^{-d/2} \int_{\mathcal{S}} \psi(\mathbf{x})f(\mathbf{x})d\mathbf{x} + \lambda^2 \int_{\mathcal{S}} b^2(\mathbf{x})d\mathbf{x} \right] + o(n^{-4/(d+4)}). \quad (3.16)$$

Theorem 3.5 (Uniform strong consistency). Assume (3.1). If $2 \leq m \leq n/\log n$ as $m, n \rightarrow \infty$, then

$$\begin{aligned} \|f_m - f\|_{\infty} &= \mathcal{O}(m^{-1/2}), \quad \text{a.s.}, \\ \|\hat{f}_{n,m} - f\|_{\infty} &= \mathcal{O}(m^{d-1/2}\alpha_n) + \mathcal{O}(m^{-1/2}), \quad \text{a.s.} \end{aligned} \quad (3.17)$$

In particular, if $m^{2d-1} = o(n/\log n)$, then $\|\hat{f}_{n,m} - f\|_{\infty} \rightarrow 0$ a.s.

Theorem 3.6 (Asymptotic normality). Assume (3.1). Let $\mathbf{x} \in \text{Int}(\mathcal{S})$ be such that $f(\mathbf{x}) > 0$. If $n^{1/2}m^{-d/4} \rightarrow \infty$ as $m, n \rightarrow \infty$, then

$$n^{1/2}m^{-d/4}(\hat{f}_{n,m}(\mathbf{x}) - f_m(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \psi(\mathbf{x})f(\mathbf{x})). \quad (3.18)$$

If we also have $n^{1/2}m^{-d/4-1/2} \rightarrow 0$ as $m, n \rightarrow \infty$, then Theorem 3.5 implies

$$n^{1/2}m^{-d/4}(\hat{f}_{n,m}(\mathbf{x}) - f(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \psi(\mathbf{x})f(\mathbf{x})). \quad (3.19)$$

Independently of the above rates for n and m , if we assume (3.2) instead and $n^{2/(d+4)}m^{-1} \rightarrow \lambda$ for some $\lambda > 0$ as $m, n \rightarrow \infty$, then Proposition 3.1 implies

$$n^{2/(d+4)}(\hat{f}_{n,m}(\mathbf{x}) - f(\mathbf{x})) \xrightarrow{\mathcal{D}} \mathcal{N}(\lambda b(\mathbf{x}), \lambda^{-d/2}\psi(\mathbf{x})f(\mathbf{x})). \quad (3.20)$$

Remark 3.7. The rate of convergence for the d -dimensional kernel density estimator with i.i.d. data and bandwidth h is $\mathcal{O}(n^{-1/2}h^{-d/2})$ in Theorem 3.1.15 of Prakasa Rao (1983), whereas our estimator $\hat{f}_{n,m}$ converges at a rate of $\mathcal{O}(n^{-1/2}m^{d/4})$. Hence, the relation between the scaling factor m of $\hat{f}_{n,m}$ and the bandwidth h of other multivariate kernel smoothers is $m \approx h^{-2}$.

4. Proof of the results for the c.d.f. estimator $F_{n,m}^*$

Proof of Proposition 2.1. We generalize the proof of (Lorentz, 1986, Section 1.6.1), which treated the case $d = 1$. By the assumption (2.1), a second order mean value theorem yields

$$\begin{aligned} F(\mathbf{k}/m) - F(\mathbf{x}) &= \sum_{i=1}^d (k_i/m - x_i) \frac{\partial}{\partial x_i} F(\mathbf{x}) \\ &\quad + \frac{1}{2} \sum_{i,j=1}^d (k_i/m - x_i)(k_j/m - x_j) \frac{\partial^2}{\partial x_i \partial x_j} F(\boldsymbol{\xi}_{\mathbf{k}}), \end{aligned} \quad (4.1)$$

for some random vector $\boldsymbol{\xi}_{\mathbf{k}} \in \mathcal{S}$ on the line segment joining \mathbf{k}/m and \mathbf{x} . Using the well-known identities

$$\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (k_i/m - x_i) P_{\mathbf{k},m}(\mathbf{x}) = 0, \quad (4.2)$$

and

$$\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (k_i/m - x_i)(k_j/m - x_j) P_{\mathbf{k},m}(\mathbf{x}) = \frac{1}{m} (x_i \mathbb{1}_{\{i=j\}} - x_i x_j), \quad (4.3)$$

we can multiply (4.1) by $P_{\mathbf{k},m}(\mathbf{x})$ and sum over $\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}$ to obtain

$$\begin{aligned} F_m^*(\mathbf{x}) - F(\mathbf{x}) &= \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (F(\mathbf{k}/m) - F(\mathbf{x})) P_{\mathbf{k},m}(\mathbf{x}) \\ &= \frac{1}{2m} \sum_{i,j=1}^d (x_i \mathbb{1}_{\{i=j\}} - x_i x_j) \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}) \\ &\quad + \frac{1}{2} \sum_{i,j=1}^d \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (k_i/m - x_i)(k_j/m - x_j) \left(\frac{\partial^2}{\partial x_i \partial x_j} F(\boldsymbol{\xi}_{\mathbf{k}}) - \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}) \right) P_{\mathbf{k},m}(\mathbf{x}). \end{aligned} \quad (4.4)$$

To conclude, we need to show that the last term is $o(m^{-1})$. By the uniform continuity of the second order partial derivatives of F , we know that $\max_{1 \leq i,j \leq d} \|\frac{\partial^2}{\partial x_i \partial x_j} F\|_{\infty} \leq M_d$ for some $M_d > 0$, and we also know that, for all $\varepsilon > 0$, there exists $0 < \delta_{\varepsilon,d} \leq 1$ such that $\|\mathbf{y} - \mathbf{x}\|_1 \leq \delta_{\varepsilon,d}$ implies $\max_{1 \leq i,j \leq d} |\frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{y}) - \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x})| \leq \varepsilon$, uniformly for $\mathbf{x}, \mathbf{y} \in \mathcal{S}$. By considering the two cases $\|\mathbf{k}/m - \mathbf{x}\|_1 \leq \delta_{\varepsilon,d}$ and $\|\mathbf{k}/m - \mathbf{x}\|_1 > \delta_{\varepsilon,d}$, the last term in (4.4) is

$$\leq \frac{1}{2} \sum_{i,j=1}^d \left[\varepsilon \sum_{\substack{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S} \\ \|\mathbf{k}/m - \mathbf{x}\|_1 \leq \delta_{\varepsilon,d}}} |k_i/m - x_i| |k_j/m - x_j| P_{\mathbf{k},m}(\mathbf{x}) + 2M_d \sum_{\ell=1}^d \sum_{\substack{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S} \\ \|k_{\ell}/m - x_{\ell}\| > \delta_{\varepsilon,d}/d}} P_{\mathbf{k},m}(\mathbf{x}) \right]. \quad (4.5)$$

By Cauchy-Schwarz and the identity (4.3), the first term inside the bracket in (4.5) is

$$\leq \varepsilon \cdot \sqrt{m^{-1} x_i (1 - x_i)} \cdot \sqrt{m^{-1} x_j (1 - x_j)} \leq \frac{\varepsilon}{4m}. \quad (4.6)$$

By Bernstein's inequality (see e.g. Lemma A.1), the second term inside the bracket in (4.5) is

$$\leq 2M_d \cdot d \cdot 2 \exp \left(- \frac{(m\delta_{\varepsilon,d}/d)^2/2}{m \cdot 1 + \frac{1}{3} \cdot 1 \cdot (m\delta_{\varepsilon,d}/d)} \right) \leq 4d M_d e^{-\delta_{\varepsilon,d}^2 m/(4d^2)}. \quad (4.7)$$

If we take a sequence $\varepsilon = \varepsilon(m) \searrow 0$ such that $1 \geq \delta_{\varepsilon(m),d} \geq m^{-1/4}$, then (4.5) is $o(m^{-1})$. \square

Proof of Theorem 2.2. The expression for the bias of $F_{n,m}^*(\mathbf{x})$ just follows from Proposition 2.1 and the fact that

$$\mathbb{E}[F_{n,m}^*(\mathbf{x})] = F_m^*(\mathbf{x}), \quad \text{for all } \mathbf{x} \in \mathcal{S}. \quad (4.8)$$

To estimate the variance of $F_{n,m}^*(\mathbf{x})$, note that

$$F_{n,m}^*(\mathbf{x}) - F_m^*(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (F_n(\mathbf{k}/m) - F(\mathbf{k}/m)) P_{\mathbf{k},m}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n Z_{i,m}, \quad (4.9)$$

where

$$Z_{i,m} := \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (\mathbb{1}_{(-\infty, \frac{\mathbf{k}}{m}]}(\mathbf{X}_i) - F(\mathbf{k}/m)) P_{\mathbf{k},m}(\mathbf{x}), \quad 1 \leq i \leq n. \quad (4.10)$$

For every m , the random variables $Z_{1,m}, \dots, Z_{n,m}$ are i.i.d. and centered, so that

$$\begin{aligned} \text{Var}(F_{n,m}^*(\mathbf{x})) &= n^{-1} \mathbb{E}[Z_{1,m}^2] \\ &= n^{-1} \left\{ \sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap m\mathcal{S}} F((\mathbf{k} \wedge \ell)/m) P_{\mathbf{k},m}(\mathbf{x}) P_{\ell,m}(\mathbf{x}) - (F_m^*(\mathbf{x}))^2 \right\}. \end{aligned} \quad (4.11)$$

Using the expansion in (4.1) and Proposition 2.1, the above is

$$= n^{-1} \cdot \left\{ \begin{aligned} &F(\mathbf{x})(1 - F(\mathbf{x})) + \mathcal{O}(m^{-1}) \\ &+ \sum_{i=1}^d \frac{\partial}{\partial x_i} F(\mathbf{x}) \sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap m\mathcal{S}} ((k_i \wedge \ell_i)/m - x_i) P_{\mathbf{k},m}(\mathbf{x}) P_{\ell,m}(\mathbf{x}) \\ &+ \sum_{i,j=1}^d \mathcal{O} \left(\sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap m\mathcal{S}} |k_i/m - x_i| |k_j/m - x_j| P_{\mathbf{k},m}(\mathbf{x}) P_{\ell,m}(\mathbf{x}) \right) \end{aligned} \right\}. \quad (4.12)$$

The double sum on the second line inside the braces is estimated in (A.10) of Lemma A.3. By Cauchy-Schwarz, the identity (4.3), and the fact that $\sum_{\ell \in \mathbb{N}_0^d \cap m\mathcal{S}} P_{\ell,m}(\mathbf{x}) = 1$, the double sum inside the big \mathcal{O} term is

$$\leq \max_{1 \leq i \leq n} \sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap m\mathcal{S}} |k_i/m - x_i|^2 P_{\mathbf{k},m}(\mathbf{x}) P_{\ell,m}(\mathbf{x}) \leq \frac{1}{m} \max_{1 \leq i \leq n} x_i(1 - x_i) \leq \frac{1}{4m}. \quad (4.13)$$

This ends the proof. \square

Proof of Theorem 2.5. By (4.12), (4.13) and (2.4), we have

$$\begin{aligned} \text{MISE}(F_{n,m}^*) &= \int_{\mathcal{S}} \left(\text{Var}(F_{n,m}^*(\mathbf{x})) + \text{Bias}[F_{n,m}^*(\mathbf{x})]^2 \right) d\mathbf{x} \\ &= n^{-1} \left[\int_{\mathcal{S}} F(\mathbf{x})(1 - F(\mathbf{x})) d\mathbf{x} + \mathcal{O}(m^{-1}) \right. \\ &\quad \left. + \sum_{i=1}^d \int_{\mathcal{S}} \frac{\partial}{\partial x_i} F(\mathbf{x}) \sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap m\mathcal{S}} ((k_i \wedge \ell_i)/m - x_i) P_{\mathbf{k},m}(\mathbf{x}) P_{\ell,m}(\mathbf{x}) d\mathbf{x} \right] \\ &\quad + m^{-2} \int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x} + o(m^{-2}). \end{aligned} \quad (4.14)$$

By the assumption (2.1), the partial derivatives $(\frac{\partial}{\partial x_i} F)_{i=1}^d$ are bounded on \mathcal{S} , so Lemma A.3 and the bounded convergence theorem imply

$$\begin{aligned} \text{MISE}(F_{n,m}^*) &= n^{-1} \int_{\mathcal{S}} F(\mathbf{x})(1 - F(\mathbf{x})) d\mathbf{x} - n^{-1} m^{-1/2} \int_{\mathcal{S}} \sum_{i=1}^d \frac{\partial}{\partial x_i} F(\mathbf{x}) \sqrt{\frac{x_i(1 - x_i)}{\pi}} d\mathbf{x} \\ &\quad + m^{-2} \int_{\mathcal{S}} B^2(\mathbf{x}) d\mathbf{x} + o(n^{-1} m^{-1/2}) + o(m^{-2}). \end{aligned} \quad (4.15)$$

This ends the proof. \square

Proof of Theorem 2.6. Recall from (4.9) that $F_{n,m}^*(\mathbf{x}) - F_m^*(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n Z_{i,m}$ where the $Z_{i,m}$'s are i.i.d. and centered random variables. Therefore, it suffices to show the following Lindeberg condition for double arrays:² For every $\varepsilon > 0$,

$$s_m^{-2} \mathbb{E}[Z_{1,m}^2 \mathbb{1}_{\{|Z_{1,m}| > \varepsilon n^{1/2} s_m\}}] \longrightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (4.16)$$

where $s_m^2 := \mathbb{E}[Z_{1,m}^2]$ and where $m = m(n) \rightarrow \infty$. But this follows from the fact that $|Z_{1,m}| \leq 2$ for all m , and $s_m = (n \text{Var}(F_{n,m}^*))^{1/2} \rightarrow \sigma(\mathbf{x})$ as $m \rightarrow \infty$ by Theorem 2.2. \square

Before proving Theorem 2.7, we need the following lemma (it is an adaptation of Lemma 2.2 in Babu & Chaubey (2006)).

Lemma 4.1. *Let F be Lipschitz continuous on \mathcal{S} , and let³*

$$N_{\mathbf{x},m} := \left\{ \mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S} : \max_{1 \leq i \leq d} \left| \frac{k_i}{m} - x_i \right| \leq \alpha_m \right\}. \quad (4.17)$$

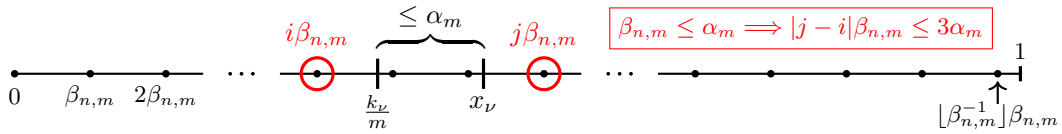
Then, for all $m \geq 2$ that satisfies $m^{-1} \leq \beta_{n,m} \leq \alpha_m$, we have, as $n \rightarrow \infty$,

$$\sup_{\mathbf{x} \in \text{Int}(\mathcal{S})} \max_{\mathbf{k} \in N_{\mathbf{x},m}} |F_n(\mathbf{k}/m) - F(\mathbf{k}/m) - F_n(\mathbf{x}) + F(\mathbf{x})| = \mathcal{O}(\beta_{n,m}) \quad \text{a.s.} \quad (4.18)$$

Proof. For all $\mathbf{k} \in N_{\mathbf{x},m}$, we have

$$\begin{aligned} & |F_n(\mathbf{k}/m) - F(\mathbf{k}/m) - F_n(\mathbf{x}) + F(\mathbf{x})| \\ & \leq \sum_{\nu=1}^d \left| F_n\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, \frac{k_{\nu}}{m}, x_{\nu+1}, \dots, x_d\right) - F\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, \frac{k_{\nu}}{m}, x_{\nu+1}, \dots, x_d\right) \right. \\ & \quad \left. - F_n\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, x_{\nu}, x_{\nu+1}, \dots, x_d\right) + F\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, x_{\nu}, x_{\nu+1}, \dots, x_d\right) \right| \\ & \leq \sum_{\nu=1}^d \max_{\substack{i,j \in \mathbb{N}_0 : \\ |i-j|\beta_{n,m} \leq 3\alpha_m}} \left| \begin{aligned} & F_n\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, j\beta_{n,m}, x_{\nu+1}, \dots, x_d\right) \\ & - F\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, j\beta_{n,m}, x_{\nu+1}, \dots, x_d\right) \\ & - F_n\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, i\beta_{n,m}, x_{\nu+1}, \dots, x_d\right) \\ & + F\left(\frac{k_1}{m}, \dots, \frac{k_{\nu-1}}{m}, i\beta_{n,m}, x_{\nu+1}, \dots, x_d\right) \end{aligned} \right| + \mathcal{O}(\beta_{n,m}), \end{aligned} \quad (4.19)$$

where the last inequality comes from our assumption that F is Lipschitz continuous.



For $\ell_{\nu}\beta_{n,m} < y_{\nu} \leq (\ell_{\nu} + 1)\beta_{n,m}$, $\nu = 1, 2, \dots, d$, and using the notation $\ell_{\nu}^+ = \ell_{\nu} + 1$, we have

$$\begin{aligned} & \left| F_n(y_1, \dots, y_{\nu-1}, j\beta_{n,m}, y_{\nu+1}, \dots, y_d) - F(y_1, \dots, y_{\nu-1}, j\beta_{n,m}, y_{\nu+1}, \dots, y_d) \right. \\ & \quad \left. - F_n(y_1, \dots, y_{\nu-1}, i\beta_{n,m}, y_{\nu+1}, \dots, y_d) + F(y_1, \dots, y_{\nu-1}, i\beta_{n,m}, y_{\nu+1}, \dots, y_d) \right| \\ & \leq \left| \begin{aligned} & F_n(\ell_1^+ \beta_{n,m}, \dots, \ell_{\nu-1}^+ \beta_{n,m}, j\beta_{n,m}, \ell_{\nu+1}^+ \beta_{n,m}, \dots, \ell_d^+ \beta_{n,m}) \\ & - F(\ell_1 \beta_{n,m}, \dots, \ell_{\nu-1} \beta_{n,m}, j\beta_{n,m}, \ell_{\nu+1} \beta_{n,m}, \dots, \ell_d \beta_{n,m}) \\ & - F_n(\ell_1 \beta_{n,m}, \dots, \ell_{\nu-1} \beta_{n,m}, i\beta_{n,m}, \ell_{\nu+1} \beta_{n,m}, \dots, \ell_d \beta_{n,m}) \\ & + F(\ell_1^+ \beta_{n,m}, \dots, \ell_{\nu-1}^+ \beta_{n,m}, i\beta_{n,m}, \ell_{\nu+1}^+ \beta_{n,m}, \dots, \ell_d^+ \beta_{n,m}) \end{aligned} \right| \end{aligned}$$

²See e.g. Section 1.9.3. in Serfling (1980).

³You can think of $N_{\mathbf{x},m}$ as the bulk of the Multinomial(m, \mathbf{x}) distribution; the contributions coming from outside the bulk are small for appropriate α_m 's.

$$\begin{aligned}
&\leq \left| \begin{aligned} &F_n(\ell_1^+ \beta_{n,m}, \dots, \ell_{\nu-1}^+ \beta_{n,m}, j \beta_{n,m}, \ell_{\nu+1}^+ \beta_{n,m}, \dots, \ell_d^+ \beta_{n,m}) \\ &- F_n(\ell_1 \beta_{n,m}, \dots, \ell_{\nu-1} \beta_{n,m}, i \beta_{n,m}, \ell_{\nu+1} \beta_{n,m}, \dots, \ell_d \beta_{n,m}) \\ &- F(\ell_1^+ \beta_{n,m}, \dots, \ell_{\nu-1}^+ \beta_{n,m}, j \beta_{n,m}, \ell_{\nu+1}^+ \beta_{n,m}, \dots, \ell_d^+ \beta_{n,m}) \\ &+ F(\ell_1 \beta_{n,m}, \dots, \ell_{\nu-1} \beta_{n,m}, i \beta_{n,m}, \ell_{\nu+1} \beta_{n,m}, \dots, \ell_d \beta_{n,m}) \end{aligned} \right| + \mathcal{O}(\beta_{n,m}) \\
&\leq \sum_{\nu=1}^d D_{n,m,\nu} + \mathcal{O}(\beta_{n,m}), \tag{4.20}
\end{aligned}$$

where

$$\begin{aligned}
D_{n,m,\nu} := & \max_{\substack{i,j \in \mathbb{N}_0: \\ |i-j| \beta_{n,m} \leq 3\alpha_m}} \max_{\substack{0 \leq k_p \leq 1 + \lfloor \beta_{n,m}^{-1} \rfloor \\ p \in \{1,2,\dots,d\} \setminus \{\nu\}}} \left| \begin{aligned} &F_n(k_1 \beta_{n,m}, \dots, k_{\nu-1} \beta_{n,m}, j \beta_{n,m}, k_{\nu+1} \beta_{n,m}, \dots, k_d \beta_{n,m}) \\ &- F_n(k_1 \beta_{n,m}, \dots, k_{\nu-1} \beta_{n,m}, i \beta_{n,m}, k_{\nu+1} \beta_{n,m}, \dots, k_d \beta_{n,m}) \\ &- F(k_1 \beta_{n,m}, \dots, k_{\nu-1} \beta_{n,m}, j \beta_{n,m}, k_{\nu+1} \beta_{n,m}, \dots, k_d \beta_{n,m}) \\ &+ F(k_1 \beta_{n,m}, \dots, k_{\nu-1} \beta_{n,m}, i \beta_{n,m}, k_{\nu+1} \beta_{n,m}, \dots, k_d \beta_{n,m}) \end{aligned} \right|. \tag{4.21}
\end{aligned}$$

By (4.19), it follows that

$$\sup_{\mathbf{x} \in \text{Int}(\mathcal{S})} \max_{\mathbf{k} \in N_{\mathbf{x},m}} |F_n(\mathbf{k}/m) - F(\mathbf{k}/m) - F_n(\mathbf{x}) + F(\mathbf{x})| \leq d \sum_{\nu=1}^d D_{n,m,\nu} + \mathcal{O}(\beta_{n,m}). \tag{4.22}$$

We want to apply a concentration bound on each $D_{n,m,\nu}$, $\nu = 1, 2, \dots, d$. By Bernstein's inequality (see e.g. Lemma A.1), note that for any $\rho > 0$, any $y_1, \dots, y_{\nu-1}, y_{\nu+1}, \dots, y_d \in \mathbb{R}$ and any $i, j \in \mathbb{N}_0$ such that $|i - j| \beta_{n,m} \leq 3\alpha_m$, we have, assuming that $\beta_{n,m} \leq \alpha_m$,

$$\begin{aligned}
&\mathbb{P} \left(\left| \begin{aligned} &F_n(y_1, \dots, y_{\nu-1}, j \beta_{n,m}, y_{\nu+1}, \dots, y_d) \\ &- F_n(y_1, \dots, y_{\nu-1}, i \beta_{n,m}, y_{\nu+1}, \dots, y_d) \\ &- F(y_1, \dots, y_{\nu-1}, j \beta_{n,m}, y_{\nu+1}, \dots, y_d) \\ &+ F(y_1, \dots, y_{\nu-1}, i \beta_{n,m}, y_{\nu+1}, \dots, y_d) \end{aligned} \right| \geq \rho \beta_{n,m} \right) \\
&\leq 2 \exp \left(- \frac{\rho^2 n^2 \beta_{n,m}^2 / 2}{n \cdot C \cdot 3\alpha_m + \frac{1}{3} \cdot 1 \cdot \rho n \beta_{n,m}} \right) \leq 2n^{-\rho^2/(8C)}, \tag{4.23}
\end{aligned}$$

where $C \geq \rho$ is a Lipschitz constant for F . A union bound over i, j and the k_p 's then yields

$$\mathbb{P}(D_{n,m,\nu} > \rho \beta_{n,m}) \leq (2 + \lfloor \beta_{n,m}^{-1} \rfloor)^{2+(d-1)} \cdot 2n^{-\rho^2/(8C)}, \quad 1 \leq \nu \leq d. \tag{4.24}$$

Since $b_{n,m}^{-1} \leq n^2$ (indeed, our assumption $m^{-1} \leq b_{n,m}$ implies $b_{n,m}^{-1} \leq m$, and the second assumption $b_{n,m} \leq \alpha_m$ implies $m \leq n^2$), we can choose a constant $\rho = \rho(C, d) > 0$ large enough that the right-hand side of (4.24) is summable in n , in which case the Borel-Cantelli lemma implies $D_{n,m,\nu} = \mathcal{O}(\beta_{n,m})$ a.s. as $n \rightarrow \infty$. The conclusion follows from the bound in (4.22). \square

Proof of Theorem 2.7. By the triangle inequality and $\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} P_{\mathbf{k},m}(\mathbf{x}) = 1$, we have

$$\begin{aligned}
\|F_{n,m}^* - F\|_{\infty} &\leq \|F_{n,m}^* - F\|_{\infty} + \|F_m^* - F\|_{\infty} \\
&\leq \|F_n - F\|_{\infty} + \|F_m^* - F\|_{\infty}. \tag{4.25}
\end{aligned}$$

The first term on the last line goes to 0 by the Glivenko-Cantelli theorem, and the second term goes to 0 by the multidimensional Bernstein's theorem (i.e. a weak version of Proposition 2.1 where F is only assumed to be continuous on \mathcal{S}).⁴

⁴To be more precise, on the first line of (4.4), use the uniform continuity of F inside the bulk $N_{\mathbf{x},m}$ and a concentration bound to show that the contributions coming from outside the bulk are negligible. Alternatively, see Theorem 1.1.1 in Lorentz (1986).

For the remainder of the proof, we study the closeness between $F_{n,m}^*$ and the empirical cumulative distribution function F_n . We assume that F is differentiable on \mathcal{S} and its partial derivatives are Lipschitz continuous. By the triangle inequality,

$$\begin{aligned} \|F_{n,m}^* - F_n\|_\infty &\leq \left\| \sum_{\mathbf{k} \in N_{\mathbf{x},m}} (F_n(\mathbf{k}/m) - F(\mathbf{k}/m) - F_n(\cdot) + F(\cdot)) P_{\mathbf{k},m}(\cdot) \right\|_\infty \\ &\quad + \left\| \sum_{\mathbf{k} \in (\mathbb{N}_0^d \cap m\mathcal{S}) \setminus N_{\mathbf{x},m}} (F_n(\mathbf{k}/m) - F(\mathbf{k}/m) - F_n(\cdot) + F(\cdot)) P_{\mathbf{k},m}(\cdot) \right\|_\infty \\ &\quad + \left\| \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}} (F(\mathbf{k}/m) - F(\cdot)) P_{\mathbf{k},m}(\cdot) \right\|_\infty. \end{aligned} \quad (4.26)$$

The first norm is $\mathcal{O}(\beta_{n,m})$ by Lemma 4.1 (assuming $m^{-1} \leq \beta_{n,m} \leq \alpha_m$). If $X_i \sim \text{Binomial}(m, x_i)$, then a union bound, the fact that $\max_{\mathbf{k}} \|F_n(\mathbf{k}/m) - F(\cdot)\|_\infty \leq 1$, and Bernstein's inequality (see e.g. Lemma A.1), yield that the second norm in (4.26) is

$$\begin{aligned} &\leq 2 \cdot \max_{\mathbf{x} \in \mathcal{S}} \sum_{i=1}^d \mathbb{P}(|X_i - mx_i| \geq m\alpha_m) \leq \max_{\mathbf{x} \in \mathcal{S}} 4 \exp \left(- \frac{m^2 \alpha_m^2 / 2}{m \cdot x_i(1-x_i) + \frac{1}{3} \cdot 1 \cdot m\alpha_m} \right) \\ &\leq 4m^{-1} \leq 4\beta_{n,m}. \end{aligned} \quad (4.27)$$

For the third norm in (4.26), the Lipschitz continuity of the partial derivatives $(\frac{\partial}{\partial x_i} F)_{i=1}^d$ implies that, uniformly for $\mathbf{x} \in \mathcal{S}$,

$$F(\mathbf{k}/m) - F(\mathbf{x}) = \sum_{i=1}^d (k_i/m - x_i) \frac{\partial}{\partial x_i} F(\mathbf{x}) + \sum_{i,j=1}^d \mathcal{O}(|k_i/m - x_i| |k_j/m - x_j|). \quad (4.28)$$

After multiplying (4.28) by $P_{\mathbf{k},m}(\mathbf{x})$, summing over $\mathbf{k} \in \mathbb{N}_0^d \cap m\mathcal{S}$ and applying the Cauchy-Schwarz inequality, the result is uniformly bounded by $\mathcal{O}(m^{-1})$ because of the identities (4.2) and (4.3). Since we assumed $m^{-1} \leq \beta_{n,m}$, this ends the proof. \square

5. Proof of the results for the density estimator $\hat{f}_{n,m}$

Proof of Proposition 3.1. We follow the proof of Proposition 2.1. Using Taylor expansions for any \mathbf{k} such that $\|\mathbf{k}/m - \mathbf{x}\|_1 = o(1)$, we obtain

$$\begin{aligned} &m^d \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} - f(\mathbf{x}) \\ &= f(\mathbf{k}/m) - f(\mathbf{x}) + \frac{1}{2m} \sum_{i=1}^d \frac{\partial}{\partial x_i} f(\mathbf{k}/m) + \mathcal{O}(m^{-2}) \\ &= \frac{1}{m} \sum_{i=1}^d \frac{\partial}{\partial x_i} f(\mathbf{x}) (k_i - mx_i) + \frac{1}{2m} \sum_{i=1}^d \frac{\partial}{\partial x_i} f(\mathbf{x}) + o(m^{-1}) \\ &\quad + \frac{1}{2m^2} \sum_{i,j=1}^d \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x}) (k_i - mx_i) (k_j - mx_j) (1 + o(1)) \\ &= \frac{1}{m} \sum_{i=1}^d \frac{\partial}{\partial x_i} f(\mathbf{x}) (k_i - (m-1)x_i) + \frac{1}{m} \sum_{i=1}^d \left(\frac{1}{2} - x_i\right) \frac{\partial}{\partial x_i} f(\mathbf{x}) \\ &\quad + \frac{1}{2m^2} \sum_{i,j=1}^d \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x}) (k_i - mx_i) (k_j - mx_j) (1 + o(1)) + o(m^{-1}). \end{aligned} \quad (5.1)$$

If we multiply the last expression by $P_{\mathbf{k},m-1}(\mathbf{x})$ and sum over $\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}$, then the identities (4.2) and (4.3) yield

$$\begin{aligned} f_m(\mathbf{x}) - f(\mathbf{x}) &= 0 + \frac{1}{m} \sum_{i=1}^d \left(\frac{1}{2} - x_i\right) \frac{\partial}{\partial x_i} f(\mathbf{x}) + \frac{1}{2m} \sum_{i,j=1}^d (x_i \mathbb{1}_{\{i=j\}} - x_i x_j) \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x}) + o(1), \end{aligned} \quad (5.2)$$

assuming that the $o(1)$ rate in $\|\mathbf{k}/m - \mathbf{x}\|_1 = o(1)$ decays slowly enough to 0 that the contributions coming from outside the bulk are negligible (exactly as we did in (4.7)). \square

Proof of Theorem 3.2. The expression for the bias is a trivial consequence of Proposition 3.1 and the fact that $\mathbb{E}[\hat{f}_{n,m}(\mathbf{x})] = f_m(\mathbf{x})$. In order to compute the asymptotics of the variance, we only assume that f is Lipschitz continuous on \mathcal{S} . First, note that

$$\hat{f}_{n,m}(\mathbf{x}) - f_m(\mathbf{x}) = \frac{m^d}{n} \sum_{i=1}^n Y_{i,m}, \quad (5.3)$$

where

$$Y_{i,m} := \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} \left[\mathbb{1}_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]}(\mathbf{X}_i) - \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} \right] P_{\mathbf{k},m-1}(\mathbf{x}), \quad 1 \leq i \leq n. \quad (5.4)$$

For every m , the random variables $Y_{1,m}, \dots, Y_{n,m}$ are i.i.d. and centered, so

$$\mathbb{V}\text{ar}(\hat{f}_{n,m}(\mathbf{x})) = n^{-1} m^{2d} \mathbb{E}[Y_{1,m}^2], \quad (5.5)$$

and it is easy to see that

$$\mathbb{E}[Y_{1,m}^2] = \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} P_{\mathbf{k},m-1}^2(\mathbf{x}) - \left(m^{-d} f_m(\mathbf{x})\right)^2. \quad (5.6)$$

The second term on the right-hand side of (5.6) is $\mathcal{O}(m^{-2d})$ since the Lipschitz continuity of f and the identity (4.3) imply that, uniformly for $\mathbf{x} \in \mathcal{S}$,

$$f_m(\mathbf{x}) - f(\mathbf{x}) = \sum_{i=1}^d \mathcal{O}\left(\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-d)\mathcal{S}} |k_i/m - x_i| P_{\mathbf{k},m-1}(\mathbf{x})\right) + \mathcal{O}(m^{-1}) = \mathcal{O}(m^{-1/2}). \quad (5.7)$$

For the first term on the right-hand side of (5.6), the Lipschitz continuity of f implies,

$$m^d \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} = f(\mathbf{k}/m) + \mathcal{O}(m^{-1}) = f(\mathbf{x}) + \mathcal{O}(m^{-1}) + \sum_{i=1}^d \mathcal{O}(|k_i/m - x_i|), \quad (5.8)$$

and by the Cauchy-Schwarz inequality, the identity (4.3) and (A.3) in Lemma A.2, we have, for all $i \in \{1, 2, \dots, d\}$,

$$\begin{aligned} &\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} |k_i/m - x_i| P_{\mathbf{k},m-1}^2(\mathbf{x}) \\ &\leq \sqrt{\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} |k_i/m - x_i|^2 P_{\mathbf{k},m-1}(\mathbf{x})} \sqrt{\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} P_{\mathbf{k},m-1}^3(\mathbf{x})} = \mathcal{O}(m^{-1/2-d/2}). \end{aligned} \quad (5.9)$$

Putting (5.7), (5.8) and (5.9) together in (5.6) yields

$$m^{3d/2} \mathbb{E}[Y_{1,m}^2] = (f(\mathbf{x}) + \mathcal{O}(m^{-1})) \left[m^{d/2} \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} P_{\mathbf{k},m-1}^2(\mathbf{x}) \right] + \mathcal{O}(m^{-1/2}). \quad (5.10)$$

The result follows from (5.5) and (A.2) in Lemma A.2. \square

Proof of Theorem 3.4. In Proposition 4.2(a) of [Ouimet \(2018\)](#), it was shown, using the duplication formula for the Γ function and the ChuVandermonde convolution for binomial coefficients, that

$$m^{d/2} \int_{\mathcal{S}} \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} P_{\mathbf{k},m-1}^2(\mathbf{x}) d\mathbf{x} = \int_{\mathcal{S}} \psi(\mathbf{x}) d\mathbf{x} + \mathcal{O}(m^{-1}). \quad (5.11)$$

Together with the almost-everywhere convergence in (A.2) of Lemma A.2, and the fact that f is bounded, Scheffé's lemma⁵ implies

$$m^{d/2} \int_{\mathcal{S}} f(\mathbf{x}) \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} P_{\mathbf{k},m-1}^2(\mathbf{x}) d\mathbf{x} = \int_{\mathcal{S}} \psi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} + o(1). \quad (5.12)$$

Therefore, by (5.5), (5.10), (5.12) and (3.6), we have

$$\begin{aligned} \text{MISE}(\hat{f}_{n,m}) &= \int_{\mathcal{S}} \left(\text{Var}(\hat{f}_{n,m}(\mathbf{x})) + \text{Bias}[\hat{f}_{n,m}(\mathbf{x})]^2 \right) d\mathbf{x} \\ &= n^{-1} m^{d/2} \int_{\mathcal{S}} \psi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} + m^{-2} \int_{\mathcal{S}} b^2(\mathbf{x}) d\mathbf{x} + o(n^{-1} m^{d/2}) + o(m^{-2}). \end{aligned} \quad (5.13)$$

This ends the proof. \square

Proof of Theorem 3.5. We have already shown that $\|f_m - f\|_{\infty} = \mathcal{O}(m^{-1/2})$ in (5.7). Next, we want to apply a concentration bound to control $\|\hat{f}_{n,m} - f_m\|_{\infty}$. Let

$$L_{n,m} := \max_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} \frac{1}{n} \sum_{i=1}^n \left(\mathbb{1}_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]}(\mathbf{X}_i) - \int_{(\frac{\mathbf{k}}{m}, \frac{\mathbf{k}+1}{m}]} f(\mathbf{y}) d\mathbf{y} \right). \quad (5.14)$$

By a union bound on $\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}$ (there are at most m^d such points), and Bernstein's inequality (see e.g. Lemma A.1), we have, for all $\rho > 0$,

$$\begin{aligned} \mathbb{P}(L_{n,m} > \rho m^{-1/2} \alpha_n) &\leq m^d \cdot 2 \exp \left(- \frac{\rho^2 n^2 m^{-1} \alpha_n^2 / 2}{n \cdot c \cdot m^{-1} + \frac{1}{3} \cdot 1 \cdot \rho n m^{-1/2} \alpha_n} \right) \\ &\leq m^d \cdot n^{-\rho^2/(4c)}, \end{aligned} \quad (5.15)$$

where the second inequality assumes that $m \leq \frac{n}{\log n}$, and $c \geq \rho$ is a Lipschitz constant for f . If we choose $\rho = \rho(c, d) > 0$ large enough, then the right-hand side of (5.15) is summable in n and the Borel-Cantelli lemma implies $\|\hat{f}_{n,m} - f_m\|_{\infty} \leq m^d L_{n,m} = \mathcal{O}(m^{d-1/2} \alpha_n)$ a.s. as $n \rightarrow \infty$. \square

Proof of Theorem 3.6. By (5.3), the asymptotic normality of $n^{1/2} m^{-d/4} (\hat{f}_{n,m}(\mathbf{x}) - f_m(\mathbf{x}))$ will follow if we verify the Lindeberg condition for double arrays:⁶ For every $\varepsilon > 0$,

$$s_m^{-2} \mathbb{E} \left[|Y_{1,m}|^2 \mathbb{1}_{\{|Y_{1,m}| > \varepsilon n^{1/2} s_m\}} \right] \rightarrow 0, \quad \text{as } n \rightarrow \infty, \quad (5.16)$$

where $s_m^2 := \mathbb{E}[|Y_{1,m}|^2]$ and $m = m(n) \rightarrow \infty$. Clearly, from (5.4),

$$|Y_{1,m}| \leq \max_{\mathbf{k} \in \mathbb{N}_0^d \cap (m-1)\mathcal{S}} 2 P_{\mathbf{k},m}(\mathbf{x}) = \mathcal{O}(m^{-d/2}), \quad (5.17)$$

and we also know that $s_m = m^{-3d/4} \sqrt{\psi(\mathbf{x}) f(\mathbf{x})} (1 + o_{\mathbf{x}}(1))$ when f is Lipschitz continuous, by the proof of Theorem 3.2, so

$$\frac{|Y_{i,m}|}{n^{1/2} s_m} = \mathcal{O}_{\mathbf{x}}(n^{-1/2} m^{-d/2} m^{3d/4}) = \mathcal{O}_{\mathbf{x}}(n^{-1/2} m^{d/4}) \rightarrow 0, \quad (5.18)$$

⁵Scheffé's lemma can be found for example on page 55 of [Williams \(1991\)](#).

⁶See e.g. Section 1.9.3. in [Serfling \(1980\)](#).

whenever $n^{1/2}m^{-d/4} \rightarrow \infty$ as $m, n \rightarrow \infty$.⁷ Under this condition, (5.16) holds and thus

$$n^{1/2}m^{-d/4}(\hat{f}_{n,m}(\mathbf{x}) - f_m(\mathbf{x})) = n^{1/2}m^{3d/4} \cdot \frac{1}{n} \sum_{i=1}^n Y_{i,m} \xrightarrow{\mathcal{D}} \mathcal{N}(0, f(\mathbf{x})\psi(\mathbf{x})). \quad (5.19)$$

This completes the proof of Theorem 3.6. \square

A. Tools

The first lemma is a standard (but very useful) concentration bound, found for example in Corollary 2.11 of [Boucheron et al. \(2013\)](#).

Lemma A.1 (Bernstein's inequality). *Let X_1, X_2, \dots, X_n be a sequence of independent random variables such that $|X_i| \leq b < \infty$. Then, for all $t > 0$,*

$$\mathbb{P}\left(\sum_{i=1}^n (X_i - \mathbb{E}[X_i]) \geq t\right) \leq 2 \exp\left(-\frac{t^2/2}{\sum_{i=1}^n \mathbb{E}[X_i^2] + \frac{1}{3}bt}\right). \quad (A.1)$$

In the second lemma, we estimate sums of powers of multinomial probabilities. This is used in the proof of Theorem 3.2 and the proof of Theorem 3.4.

Lemma A.2. *For every $\mathbf{x} \in \text{Int}(\mathcal{S})$, we have, as $r \rightarrow \infty$,*

$$r^{d/2} \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} P_{\mathbf{k},r}^2(\mathbf{x}) = [(4\pi)^d x_1 x_2 \dots x_d (1 - \|\mathbf{x}\|_1)]^{-1/2} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}), \quad (A.2)$$

$$r^d \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} P_{\mathbf{k},r}^3(\mathbf{x}) = [(2\sqrt{3}\pi)^d x_1 x_2 \dots x_d (1 - \|\mathbf{x}\|_1)]^{-1} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}). \quad (A.3)$$

Proof. It is well known that the covariance matrix of the multinomial distribution is $r \Sigma_{\mathbf{x}}$, where $\Sigma_{\mathbf{x}} = \text{diag}(\mathbf{x}) - \mathbf{x}\mathbf{x}^\top$, see e.g. ([Severini, 2005](#), p.377), and it is also known that

$$\det(\Sigma_{\mathbf{x}}) = x_1 x_2 \dots x_d (1 - \|\mathbf{x}\|_1), \quad (A.4)$$

see e.g. ([Tanabe & Sagae, 1992](#), Theorem 1). Therefore, consider

$$\phi_{\Sigma_{\mathbf{x}}}(\mathbf{y}) := \frac{1}{\sqrt{(2\pi)^d \det(\Sigma_{\mathbf{x}})}} \cdot \exp\left(-\frac{1}{2}\mathbf{y}^\top \Sigma_{\mathbf{x}}^{-1} \mathbf{y}\right), \quad \mathbf{y} \in \mathbb{R}^d, \quad (A.5)$$

the density of the multivariate normal $\mathcal{N}(\mathbf{0}, \Sigma_{\mathbf{x}})$. By a local limit theorem for the multinomial distribution (see e.g. Lemma 2 in [Arenbaev \(1976\)](#) or Theorem 2.1 in [Ouimet \(2020b\)](#)), we have

$$\begin{aligned} r^{d/2} \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} P_{\mathbf{k},r}^2(\mathbf{x}) &= \int_{\mathbb{R}^d} \phi_{\Sigma_{\mathbf{x}}}^2(\mathbf{y}) d\mathbf{y} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\ &= \frac{2^{-d/2}}{\sqrt{(2\pi)^d \det(\Sigma_{\mathbf{x}})}} \int_{\mathbb{R}^d} \phi_{\frac{1}{2}\Sigma_{\mathbf{x}}}(\mathbf{y}) d\mathbf{y} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\ &= \frac{2^{-d/2}}{\sqrt{(2\pi)^d \det(\Sigma_{\mathbf{x}})}} \cdot 1 + \mathcal{O}_{\mathbf{x}}(r^{-1/2}), \end{aligned} \quad (A.6)$$

⁷The bound on $|Y_{1,m}|$ in the proof of Proposition 1 in [Babu et al. \(2002\)](#) is suboptimal when $d = 1$, this is why we get a slightly better rate in (5.18).

and

$$\begin{aligned}
r^d \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} P_{\mathbf{k},r}^3(\mathbf{x}) &= \int_{\mathbb{R}^d} \phi_{\Sigma_{\mathbf{x}}}^3(\mathbf{y}) d\mathbf{y} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\
&= \frac{3^{-d/2}}{(2\pi)^d \det(\Sigma_{\mathbf{x}})} \int_{\mathbb{R}^d} \phi_{\frac{1}{3}\Sigma_{\mathbf{x}}}(\mathbf{y}) d\mathbf{y} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\
&= \frac{3^{-d/2}}{(2\pi)^d \det(\Sigma_{\mathbf{x}})} \cdot 1 + \mathcal{O}_{\mathbf{x}}(r^{-1/2}).
\end{aligned} \tag{A.7}$$

This ends the proof. \square

In the third lemma, we estimate another technical sum, needed in proof Theorem 2.2 and the proof of Theorem 2.5.

Lemma A.3. *For $i \in \{1, 2, \dots, d\}$ and $r \in \mathbb{N}$, let*

$$R_{i,r}(\mathbf{x}) := r^{1/2} \sum_{\mathbf{k}, \ell \in \mathbb{N}_0^d \cap r\mathcal{S}} ((k_i \wedge \ell_i)/r - x_i) P_{\mathbf{k},r}(\mathbf{x}) P_{\ell,r}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{S}. \tag{A.8}$$

Then,

$$\sup_{1 \leq i \leq d} \sup_{r \in \mathbb{N}} \sup_{\mathbf{x} \in \mathcal{S}} |R_{i,r}(\mathbf{x})| \leq 1, \tag{A.9}$$

and for every $\mathbf{x} \in \text{Int}(\mathcal{S})$, we have,

$$R_{i,r}(\mathbf{x}) = -\sqrt{\frac{x_i(1-x_i)}{\pi}} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}), \quad \text{as } r \rightarrow \infty. \tag{A.10}$$

Proof. By the Cauchy-Schwarz inequality and the identity (4.3), we have

$$\begin{aligned}
|R_{i,r}(\mathbf{x})| &\leq 2r^{1/2} \sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} |k_i/r - x_i| P_{\mathbf{k},r}(\mathbf{x}) \leq 2r^{1/2} \sqrt{\sum_{\mathbf{k} \in \mathbb{N}_0^d \cap r\mathcal{S}} |k_i/r - x_i|^2 P_{\mathbf{k},r}(\mathbf{x})} \\
&\leq 2r^{1/2} \cdot \sqrt{r^{-1} x_i(1-x_i)} \leq 1.
\end{aligned} \tag{A.11}$$

For the second claim, we know that the marginal distributions of the multinomial are binomial, so if ϕ_{σ^2} denotes the density function of the $\mathcal{N}(0, \sigma^2)$ distribution, a standard local limit theorem for the binomial distribution (see e.g. [Prokhorov \(1953\)](#) or Theorem 2.1 in [Ouimet \(2020b\)](#)) and integration by parts show that

$$\begin{aligned}
R_{i,r}(\mathbf{x}) &= 2 \cdot x_i(1-x_i) \int_{-\infty}^{\infty} \frac{z}{x_i(1-x_i)} \phi_{x_i(1-x_i)}(z) \int_z^{\infty} \phi_{x_i(1-x_i)}(y) dy dz + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\
&= 2 \cdot x_i(1-x_i) \left[0 - \int_{-\infty}^{\infty} \phi_{x_i(1-x_i)}^2(z) dz \right] + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\
&= \frac{-2x_i(1-x_i)}{\sqrt{4\pi x_i(1-x_i)}} \int_{-\infty}^{\infty} \phi_{\frac{1}{2}x_i(1-x_i)}(z) dz + \mathcal{O}_{\mathbf{x}}(r^{-1/2}) \\
&= -\sqrt{\frac{x_i(1-x_i)}{\pi}} + \mathcal{O}_{\mathbf{x}}(r^{-1/2}).
\end{aligned} \tag{A.12}$$

This ends the proof. \square

Remark A.4. *The proof of (A.10) is much simpler here than the proof of Lemma 2(iv) in [Leblanc \(2012a\)](#) ($d = 1$), where a finely tuned continuity correction from [Cressie \(1978\)](#) was used to estimate the survival function instead of working with a local limit theorem directly. There is also a typo in Leblanc's paper, his function $\psi_2(x)$ should be equal to $[x(1-x)/(4\pi)]^{1/2}$ instead of $[x(1-x)/(2\pi)]^{1/2}$. As a consequence, his function $V(x)$ should be equal to $f(x)[x(1-x)/\pi]^{1/2}$ instead of $f(x)[2x(1-x)/\pi]^{1/2}$. The same error also affects the statements in [Belalia \(2016\)](#), since the proofs relied on the same estimates.*

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